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Optical and Infrared Emission From Disturbed E and F Layers

Part 1 – Theoretical Considerations

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13. ABSTRACT

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PROBLEM STATUS

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AUTHORIZATION

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I. Introduction.

The VUV radiation from a nuclear detonation ionizes a large volume of space to varying degrees depending on the distance from the detonation point. This ionized space is generally known as the UV-fireball. It is a disturbed atmosphere and tends to relax to its ambient condition. In doing so, it radiates.

This report concerns itself with the radiation spectrum in the visible and the infrared from disturbed E and F layers of the ionosphere. The dominant species of these layers are O, N_2, and O_2. However, under disturbed conditions, the ionic species of these neutrals, metastable atomic and molecular species are also formed. Atomic nitrogen, for example, is formed through the dissociative recombination of N_2^+ with an electron. Since this process is quite fast, nitrogen ions are formed during the irradiation period. The species of interest, excluding metals and metaloxides, during the irradiation period and thereafter are: N_2, $N_2(A^3\Sigma)$, N_2^+, O_2, $O_2(a^1\Delta)$, $O_2(b^1\Sigma)$, O_2^+, $O_2^+(a^4\pi)$, NO, NO^+, O, $O(^1D)$, $O(^1S)$, N, $N(^2D)$, $N(^2P)$, O^+, $O^+(^2D)$, $O^+(^2P)$, N^+, $N^+(^1D)$, $N^+(^1S)$ and, of course, N_e. These species are included in the NRL Master Deposition and Late-Time Chemistry Code which was designed to calculate the time history of the electrons and the optical output. This mixture of species constitutes a plasma with initial electron energy of a few eV.

Emission from such a plasma can be divided into line (or band) and continuum radiation.

A. Line emission arises from an electronic transition between two discrete quantum states of an atom or an atomic ion. In the case of the molecule one speaks of a band system which, in reality, consists of many discrete lines. The excited electronic or vibrational states responsible for line or band emissions arise through a variety of physical processes. These are: electron impact excitation, dissociative recombination, cascade from high states, charge exchange or neutral rearrangement.

B. Continuum emission, on the other hand, arises from the free-free transitions by electrons in the field of an ion and from the free-bound transition of a recombining electron with an ion.

II. Discrete Transitions.

To account for the discrete transitions one must know the population densities of the excited states which emit the radiation of interest. However, in reality it is prohibitive and impractical to have a rate equation for every excited state. In order to calculate the optical output, certain approximations are in order and necessary. The discrete transitions in general can be divided into optically allowed and forbidden transitions.

A. Forbidden Transitions

The NRL Master code contains almost all the metastable states of aeronomic interest which emit radiation in the visible and in infrared. These metastable states play important roles in the chemistry of the disturbed atmosphere in addition to their emissions.

Therefore, their time histories are of considerable interest. Table I gives the relevant line emissions from atomic and atomic ions. Data for this table are taken from Ref. 1. Table II, on the other hand, gives similar information for molecules. The lifetimes of (0-0) transition for the infrared and the atmospheric bands were obtained from Ref. 2 and 3, respectively.

TABLE I

Metastable State	Transition	Excitation Energy (eV)	Lifetime (sec)	Wavelength (Å)
$O(^1D)$	$O(^1D) \rightarrow O(^3P)$	1.96	140.0	6300
$O(^1S)$	$O(^1S) \rightarrow O(^1D)$	4.16	0.7	5577
$O^+(^2D)$	$O^+(^2D) \rightarrow O^+(^4S)$	3.31	3×10^4	3728
$O^+(^2P)$	$O^+(^2P) \rightarrow O^+(^2D)$	5.00	6.6	7319
$N(^2D)$	$N(^2D) \rightarrow N(^4S)$	2.37	2×10^5	5200
$N(^2P)$	$N(^2P) \rightarrow N(^2D)$	3.56	13.0	10404
$N^+(^1D)$	$N^+(^1D) \rightarrow N^+(^3P)$	1.88	8×10^4	6527
$N^+(^1S)$	$N^+(^1S) \rightarrow N^+(^1D)$	4.03	0.92	5755

TABLE II

Metastable State	Transition	Excitation Energy (eV)	Lifetime (sec)	Wavelength (μm)
$O_2(a^1\Delta)$	$a^1\Delta \rightarrow X^3\Sigma$ (0-0)	0.98	2.7×10^{3}	1.27
$O_2(b^1\Sigma)$	$b^1\Sigma \rightarrow X^3\Sigma$ (0-0)	1.6	12	0.7619

The excitation energies, on the other hand, are from Herzberg[4]. It should be emphasized that other bands also occur. For example, (0-1) band of the atmospheric system has a transition at 0.8645μ. However, the (0-0) band is stronger[5] than (0-1) band by at least an order of magnitude.

B. Allowed Transitions

The following bands of interest could be included under the allowed transitions. These are:

1. Mienel Band System of N_2^+ (A-X)

These transitions[6] are in the visible and the infrared. This band system can be excited by electron impacts with the molecular ions in their ground state. However, no such cross section has yet been measured. One may use a Seaton-type cross section with an oscillation strength $\sim 3 \times 10^{-3}$ to obtain an idea on the strength of emission due to electron excitation. One interesting method of excitation of certain bands of the Mienel system is the resonance charge exchange process

given by the reaction

$$O^+(^2D) + N_2 \longrightarrow N_2^+(A,\ v' = 1) + O \qquad (1)$$

This process may excite two interesting bands, the (1-0) with $\lambda \simeq 9212$Å and (1-2) with $\lambda \simeq 1529$Å. It should be remarked at the outset that Hinteregger[7] has observed that these bands often have anomalously high intensities in the aurora, due perhaps to reaction (1).

2. N_2^+ First Negative System

This band can be excited by electron impacts with the ground state of the ion. This cross-section has been measured[8]. However, in an experiment[9] performed at NRL to measure the rate coefficient, it was found that the above cross section may be too large, perhaps by as much as a factor of 60. Therefore, it may be necessary to readjust Lee and Carlton's cross section in order to calculate the output of the (0-0) band at 3914Å.

3. O_2^+ Second Negative Band

The zeroth vibrational level of $O_2^+(A^2\pi)$ can be excited according to the reaction

$$O^+(^2D) + O_2 \longrightarrow O_2^+(A^2\pi) + O \qquad (2)$$

Part of this band is in the visible and could be accounted for.

4. NO Infrared Emission

The following reactions form NO:

$$N + O_2 \rightarrow NO + O \qquad (3)$$

$$N(^2D) + O_2 \rightarrow NO + O \qquad (4)$$

The energy released in reaction (1) is ~ 1.4 eV and may excite the $6^{\underline{th}}$ vibrational level of NO, thus resulting in infrared emission. The chemiluminescence of reaction (1) has been investigated recently.[10] However, reaction (4) is faster than (1) and its chemiluminescence has not yet been investigated even though more energy release may be expected. Two infrared bands are expected as the results of reactions (3) and (4). These are located at 5.3 um and 2.7 um bands.

A simple steady-state solution gives the following population densities of the vibrational levels of NO in descending order starting from $v = 6$: 0.139, 0.143, 0.197, 0.277, 0.445, 0.956. These are in units of Q/A_{10}, where Q is the excitation rate for the $6^{\underline{th}}$ vibrational level and A_{10} is the transition probability for the fundamental. Here, it is assumed that the fundamental and the overtone are the only important emissions. This simple calculation results in fundamental and overtone volume intensities of 5Q and 0.48Q, respectively.

5. NO^+ Infrared Emission

The fundamental, 4.3μ, and the overtone, 2.15μ, are characteristic emissions of NO^+. These infrared emissions can be accounted for if one knows exactly the vibrational excitations of NO^+. This molecular ion is formed by the following reactions:

$$N_2^+ + O \rightarrow NO^+ + N \qquad (5)$$

$$O^+ + N \rightarrow NO^+ + N \qquad (6)$$

and

$$N^+ + O_2 \rightarrow NO^+ + O \qquad (7)$$

These reactions are all exothermic and the energy released in each reaction, assuming that the reaction products are in their ground states and do not acquire additional thermal energies, is 3.1, 1.1 and 6.6 eV, respectively. However, with these excess energies available, the reaction products may be in excited electronic states. For example, in (5) the nitrogen atom could end up in $N(^2D)$ state, thus reducing the excess energy by 2.37 eV. In Reaction (7) the oxygen atom may end up either in $O(^1D)$ or $O(^1S)$, thereby reducing the excess energy by 1.96 and 4.16, respectively. These branching ratios are not known, however, one can estimate them. Furthermore, the chemiluminescence of Reactions (4) to (6) have not been measured. Therefore, the emission from NO^+ can only be estimated at this stage of the game between some upper and a lower limit.

In addition to the above allowed transitions, a major source of the visible and the infrared radiation, especially during the late-time development, is from the bound-bound electronic transitions of highly excited atomic states. In what follows we give a general view for calculating this part of the radiation spectrum.

In principle, the power density emitted in bound-bound transitions is

$$P_{bb} = \sum_{n>n_{min}}^{n_{max}} \sum_{n_{min}=n'}^{n_{max}} N_n A_{nn'} h\nu_{nn'} \qquad (8)$$

where N_n is the population density of atoms in excited state n, $A_{nn'}$ is the spontaneous transition rate from state n to n' and $h\nu_{nn'}$ is the energy of the emitted photon. The sum in (8) theoretically should go to ∞; however, because of the advance of the series limit, a maximum n exists for a given electron density in the plasma. Since the major ion during the late time development is O^+, an approximate hydrogen like semi-classical calculation is feasible. In thermodynamic equilibrium N_n is related to the electron, N_e, and ion, N_i, densities, through Saha relation[11] as

$$N_n = N_e N_i \left(\frac{h^2}{2\pi mkT}\right)^{3/2} \frac{g_n}{2} e^{E_n/kT} \qquad (9)$$

Here g_n is the statistical weight on level n whose binding energy is $E_n = \frac{Z^2 E_H}{n^2}$. E_H is the ionization energy of H and the rest of the symbols have the usual meaning. The above expression relates N_n to the ground state population of N_i. This relation is valid for temperature ranges of interest. At higher temperatures one must use Saha equation with partition functions. Also, in the range of interest, equation (9) may not be valid and one may calculate the departure of those excited states from their thermal equilibrium values. The intensity for a transition from state n to a lower state n' is

$$I_{nn'} = N_n A_{nn'} h\nu_{nn'} \qquad (10)$$

where

$$A_{nn'} = \frac{g_{n'}}{g_n} \frac{8\pi^2 e^2 \nu_{nn'}^2}{mc^3} f_{nn'} \qquad (11)$$

Using the semi-classical expression for the oscillator strength[12] with unit Gaunt factor,

$$f_{nn'} = \frac{2^6}{3\sqrt{3}\,\pi} \frac{1}{g_{n'}} \left(\frac{1}{n'^2} - \frac{1}{n^2}\right)^{-3} \frac{1}{n^3}\frac{1}{n'^3}, \quad (12)$$

and substituting expression (9) into (10) one obtains

$$I_{nn'} = 3.245 \times 10^{-6} \frac{N_e N_i Z^4}{T^{3/2}} \frac{2hRZ^2}{n^3} \frac{1}{n'^3} \exp\left(\frac{Z^2 E_H}{n^2 kT}\right) \quad (13)$$

where the following energy relation was utilized:

$$\frac{h\nu_{nn'}}{Z^2 E_H} = \frac{1}{n'^2} - \frac{1}{n^2} \quad (14)$$

This last relation can be utilized to define the frequency of interest so that calculations of (13) can yield the bound-bound transitions. However, for higher n values one may assume continuous distribution of n.

III. Continuum Radiation.

The continuum radiation arises from free-free and free-bound electron transitions in a plasma.

A. Free-Free Transitions

The continuum emission due to free-free transitions in ergs per unit volume per unit time, using unit Gaunt factor, is[11]

$$\epsilon_{ff}(\lambda)\,d\lambda = 2.047 \times 10^{-27} \frac{\Delta\lambda}{\lambda^2} \frac{1}{\sqrt{T}} e^{-\frac{1.44}{\lambda T}} N_e N_i \quad (15)$$

B. Free-Bound Transitions

The free-bound contribution to the continuum intensity per unit volume per unit time, again using unit Gaunt factors, is[11]

$$\epsilon_{fb}(\lambda)\,d\lambda = 6.453 \times 10^{-22} \frac{N_e N_i}{T^{3/2}} \cdot \frac{\Delta\lambda}{\lambda^2} \; e^{-\frac{1.44}{\lambda T}} \sum_{n_{min}}^{n_{max}} \frac{1}{n^3} \; e^{\frac{Z^2 E_H}{n^2 kT}} \qquad (16)$$

Expressions (15) and (16) are easy to evaluate. In (16) n_{max} is defined by the advance of the series limit and n_{min} must satisfy the following relation for a given frequency

$$\hbar\omega \geq E_i - E_n \qquad (17)$$

where E_i is the ionization energy of the atom and E_n is the excitation energy of state n. Some results of the calculations of (15) and (16) are shown in Figures (1) and (2), where $\Delta\lambda = 1\,\text{Å}$ was used.

The free-bound and the free-free expressions can be derived using line smearing method from Equation (13). The line emission coefficient using (13) can be written as

$$\epsilon(\omega) = \bar{K} \frac{1}{T^{3/2}} \frac{N_e}{n^3} \frac{N_i}{n'^3} \; e^{\frac{Z^2 E_H}{n^2 kT}} \; L(\omega) \qquad (1-)$$

When $\bar{K}$ is all the relevant constants of Equation (13), E_H is the ionization energy of hydrogen atom, and $L(\omega)$ is the line shape. Assume that the line is normalized to a rectangular shape, such that $L(\omega)\ \Delta\omega = 1$. Thus, $\Delta\omega$

becomes the separation between neighboring lines of the same series, i.e., $\Delta\omega \simeq \frac{2E_H}{\hbar n^3}$. Using this expression for $L(\omega)$ and eliminating the dependence on final states in the exponential via $E_H\left(\frac{1}{n'^2} - \frac{1}{n^2}\right) = \hbar\omega$, one obtains

$$\epsilon(\omega) = \frac{\bar{K}'}{T^{3/2}} \frac{1}{n'^3} N_e N_i \, e^{\frac{Z^2 E_H}{n'^2 kT} - \frac{\hbar\omega}{kT}} \qquad (19)$$

To obtain an expression for the free-bound transitions into state n', sum over all n' up to the series limit. For free-free transitions, add an integral with limits of $X = \frac{E_H}{n_1^2}$ where n_1 is the series limit, and $X = -\infty$.

IV. Remarks.

This report gives possible sources of radiation in the optical and infrared from a UV-fireball created in the E and F regions by a nuclear detonation. Some of these sources may be important in certain parts and during a limited time in the development of the UV-fireball. Simple hydrogen-like expressions for the bound-bound, free-bound are proposed for the first generation calculation. NRL Master Deposition and Late-Time Chemistry Code carries all the species discussed in the text of this report. NRL's Simple Code, used in conjunction with MHD Codes, carries less species than the Master Code. However, certain steady-state relations can be used to calculate outputs from species not transported.

Other atmospheric species such as O_3, OH, H_2O, CO_2 and N_2O and their emissions will be considered in the next report.

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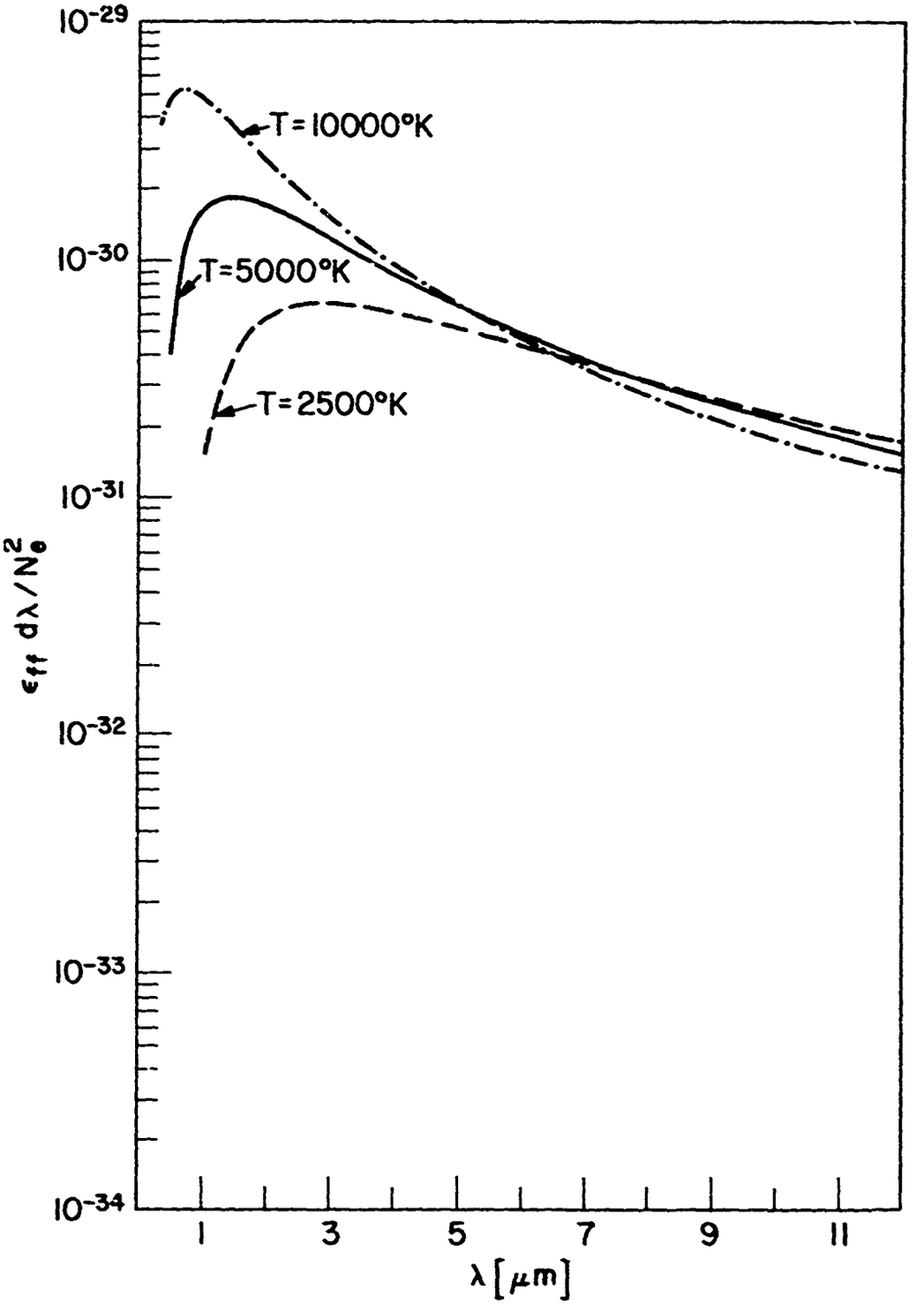
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10-30
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1
3
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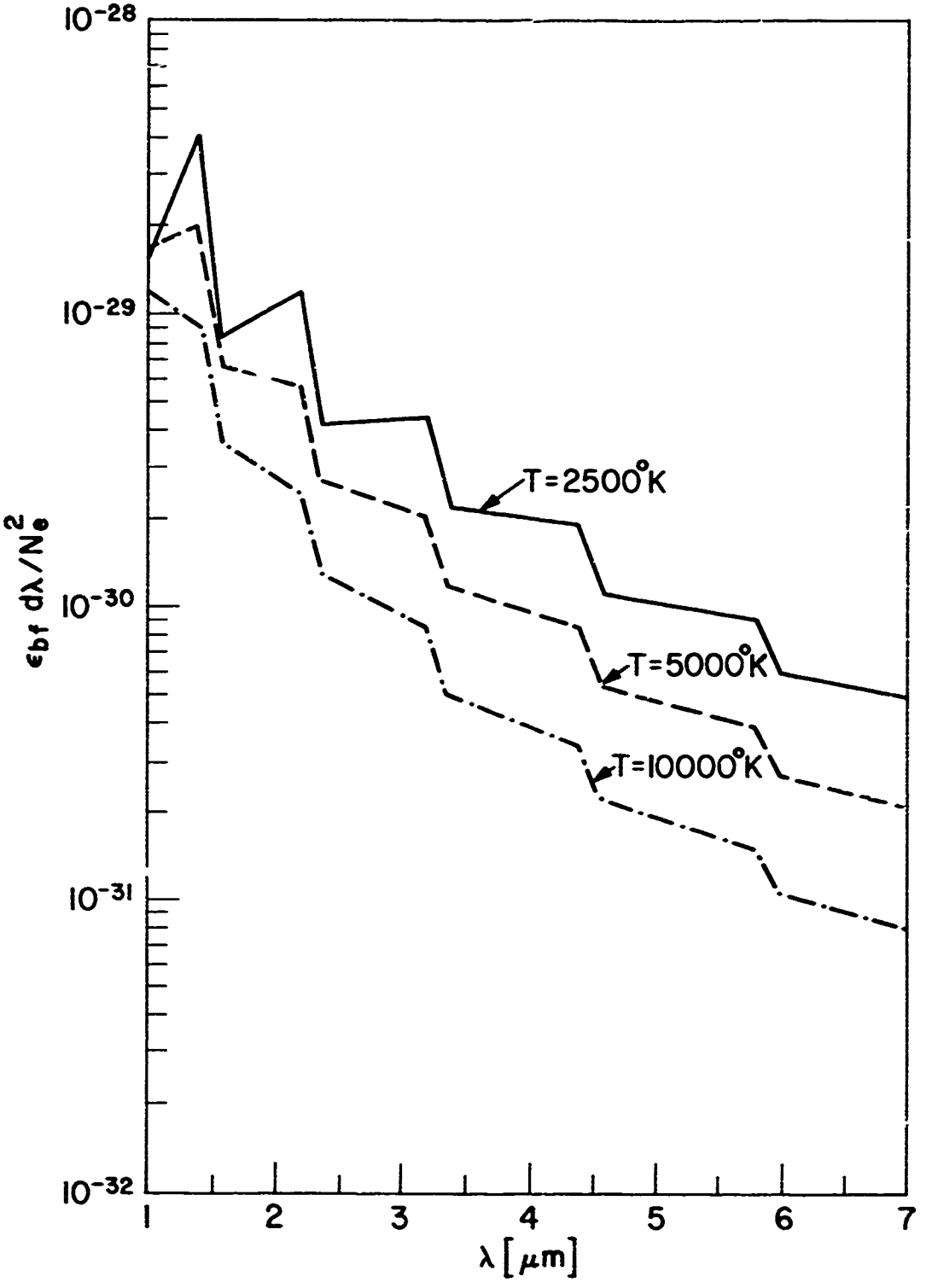
λ [μm]

Figure 1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λ [μm]

Figure 2